

## Quantum Cluster Equilibrium Theory: Carbonic Acid in the Gas and the Solid Phase

R. Ludwig

published in

*Modern Methods and Algorithms of Quantum Chemistry*,  
J. Grotendorst (Ed.), John von Neumann Institute for Computing,  
Jülich, NIC Series, Vol. 2, ISBN 3-00-005746-3, p. 10, 2000.

© 2000 by John von Neumann Institute for Computing

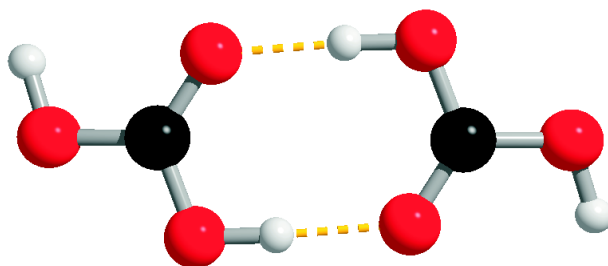
Permission to make digital or hard copies of portions of this work for personal or classroom use is granted provided that the copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise requires prior specific permission by the publisher mentioned above.

<http://www.fz-juelich.de/nic-series/>

# Quantum Cluster Equilibrium Theory: Carbonic Acid in the Gas and the Solid Phase

R. Ludwig

Physikalische Chemie, Universität Dortmund, D-44221 Dortmund,  
Germany



Despite the conventional wisdom that carbonic acid is kinetically instable, chemists recently succeeded in recognizing its stability and then in isolating and characterizing this compound. In particular, Hage et al. [1] were able to sublime and recondense carbonic acid without decomposition into carbon dioxide and water. This study could prove the stability of gas-phase carbonic acid. The vapor pressure estimates were consistent with an equilibrium mixture of monomers and dimers, comparable to that of formic acid. In this work we use the recently developed quantum cluster equilibrium (QCE) theory [2,3] at the RHF/6-31+G\* and at the B3LYP/6-31+G\* level of theory to calculate the equilibrium cluster population for carbonic acid in the gas and the solid phase. The validity of the resulting QCE model is tested by comparison with experimental thermodynamic and spectroscopic data.

- [1] W. Hage, K.R. Liedl, A. Hallbrucker, E. Mayer, *Science* **279**, 1332 (1998).
- [2] F. Weinhold, *J. Chem. Phys.* **109**, 367 (1998).
- [3] R. Ludwig, F. Weinhold, T.C. Farrar, *Ber. Bunsenges. Phys. Chem.* **102**, 197 (1998); **102**, 205 (1998).
- [4] R. Ludwig, F. Weinhold, T.C. Farrar, *Mol. Phys.* **97**, 465 (1999); **97**, 479 (1999).